

## BIDENTATE LEWIS ACIDS FOR SMALL MOLECULE ACTIVATION.

*Kudina P.I., Kazakov I.V.*<sup>1</sup>

<sup>1</sup> St. Petersburg State University, St. Petersburg, Russia

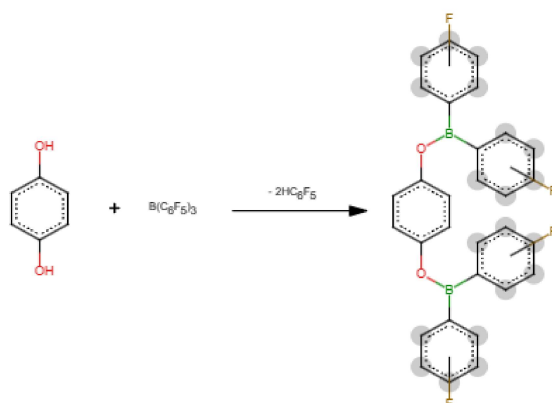
Student

[st094704@student.spbu.ru](mailto:st094704@student.spbu.ru)

Approximately 15 years ago, the concept of Frustrated Lewis Pairs (FLPs) emerged in the field of chemistry [1]. The first example was an FLP formed by tris(pentafluorophenyl)borane  $B(C_6F_5)_3$  and tritertbutylphosphine  $tBu_3P$  [1]. FLPs are unique mixtures of a potent acid and a robust Lewis base that do not form traditional adducts due to steric hindrances. This distinctive property allows FLPs to exhibit exceptional abilities in activating small molecules and chemical bonds, such as  $H_2$ ,  $CO_2$ , p-block oxides, alkenes, and alkynes as metal-free catalysts.

The reversible absorption and release of hydrogen at varying temperatures using FLPs have proven valuable, particularly in processes like the hydrogenation of olefins [2]. While FLPs based on monodentate acids have been extensively researched, those based on bidentate acids remain relatively unexplored. Bidentate Lewis acids offer the advantage of being able to coordinate two Lewis bases simultaneously, enabling reactions that were previously unattainable with monodentate acids [3].

In this study, we present a straightforward synthetic method for producing potent bidentate Lewis acids featuring the  $-OB(C_6F_5)_2$  group. Diols undergo quantitative reaction with  $B(C_6F_5)_3$  to yield the desired products through the elimination of pentafluorobenzene (Scheme 1). The reaction products of  $B(C_6F_5)_3$  with benzene-1,4-diol, benzene-1,3-diol, and ethane-1,2-diol were thoroughly characterized using NMR, IR, and mass-spectroscopy techniques. Bidentate Lewis acid structures were confirmed by single crystal X-ray diffraction.



**Scheme 1.** Synthesis of bidentate Lewis acid by interaction of benzene-1,4-diol with tris(pentafluorophenyl)borane.

Testing was conducted to evaluate the activity of bidentate Lewis acids as a component of the frustrated Lewis pair (FLP). This was achieved through their reaction with tritertbutylphosphine  $tBu_3P$  in the presence of molecular hydrogen. Notable changes were observed in the  $^1H$  and  $^{19}F$  NMR spectra, indicating the activation of  $H_2$ . This study presents a unique example of an FLP incorporating a bidentate Lewis acid.

### References

- [1] *Science* **2006**, 314, 1124–1126.
- [2] *Angew. Chem. Int. Ed.* **2012**, 51(40), 10164–10168.
- [3] *Synlett.* **2012**, 23(5), 699–705.

### Acknowledgements

This work was financially supported by the Russian Science Foundation grant 23-23-00597. The work was carried out using equipment of the resource centers of St. Petersburg State University “Centre for Magnetic Resonance” and “Centre for X-ray Diffraction Studies”.